MST e NEWS

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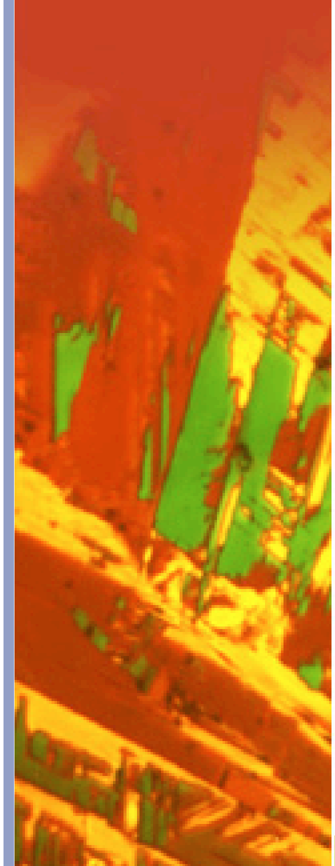

Jose 'Alfredo' Caro

Master materials scientist fills a strategic need at Los Alamos

By Francisco Ojeda
ADEPS Communications

Over the past 25 years Alfredo Caro has researched nuclear materials at government laboratories on three continents, gaining experience that has made him a successful materials scientist. In March, Caro joined Los Alamos National Laboratory as Crystal Growth and Material Preparation team leader in Structure/Property Relations (MST-8) and as a member of the Center for Materials at Irradiation and Mechanical Extremes (CMIME).

"There are always experiences and challenges in different times in your life," said Caro. "With the journey that I have taken, I felt that the time was right to take this great opportunity and continue to do some stimulating work."

Caro, who came to Los Alamos after seven years at Lawrence Livermore National Laboratory, has been a researcher at the Swiss Federal Institute of Technology and Paul Scherer Institute in Switzerland and the Instituto Balseiro in Argentina. Caro has also taught condensed matter physics and materials science at the Latin American research center and served as director of the country's Bariloche Atomic Center.

"The work was different, as was the culture and language, but there was always the same theme–my research–which helped me become comfortable quickly with the different backgrounds and cultures," said Caro, who grew up in Argentina and speaks four languages. "Experiencing so much diversity has taught me much."

Caro was drawn to Los Alamos, he said, because of the integration of his research focus with the wealth of expertise and tools available at a national laboratory.

"This is the best place to study nuclear materials research because it has so many capabilities in regards to the scientists and the facilities," he said.

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From Dave's Desk

One of my roles as Deputy Division Leader is to help define the vision for the Los Alamos signature experimental facility, MaRIE, (Matter-Radiation Interactions in Extremes). MST has several key people engaged in the facility definition: Mark Bourke (Fission Fusion materials Facility – F^3 Pillar Lead), myself (Making, Measuring, and Modeling Materials Facility – M4), and Paul Dunn (Nuclear Weapons liaison). Many other MST scientists have been involved with developing the "first experiments" that define the mission for MaRIE. These first experiments are also defining the science requirements, which ultimately drive the facility and technology requirements for MaRIE. In this "From the Desk," I'll be giving you an update on the current status of MaRIE.

Materials research is on the brink of a new era in which observation and validation of performance is replaced with prediction and control for designed functionality. LANL's solution to making the transition from observation to control is the MaRIE facility. MaRIE is proposed to be built onto the existing LANSCE facility and is focused on understanding and, ultimately, predicting the behavior of materials in extreme dynamic and irradiation environments. Materials in extreme environments are central to important mission problems for national security (stockpile materials), energy technologies (fission and fusion), and basic science (materials by design). This facility will provide improved experimental capabilities providing insights into complex material problems, e.g. fourth generation light sources, irradiation facilities, and novel in situ probes for characterization and control of materials synthesis. Simulation capabilities are providing remarkable insights at length and time scales previously inaccessible. New capabilities will be needed to realize the vision of MaRIE, e.g. in situ, dynamic measurements with simultaneous scattering and imaging, well-controlled and characterized materials using advanced synthesis and characterization, and extreme environments (dynamic loading and irradiation). All of this needs to be coupled with predictive modeling and simulation to enable materials design and discovery.

'MaRIE needs your ideas to help define and develop the novel tools that will allow us to make the transition from observation to control.'

The past few months have been an important and critical time for MaRIE. Several developments have occurred and are in progress indicating significant support for the future of MaRIE. In March, the four Under Secretaries of the Department of Energy issued a letter to LANL affirming their commitment to LANSCE for the next decade and requested LANL to develop a strategy for long-term science facility development. Director Anastasio responded in July with a LANSCE risk mitigation plan and the proposal that MaRIE is the long-term science facility solution. Recently Director Anastasio, Principal Associate Director for Science, Technology and Engineering Terry Wallace and MaRIE Capture Manager John Sarrao briefed Secretary of Energy Steven Chu and Under Secretary of Science Steven Koonin, receiving positive support for the MaRIE concept. We are gaining momentum behind MaRIE and are close to submitting a CD-0 package per recent dialogue.

How can you help? MaRIE needs your ideas to help define and develop the novel tools that will allow us to make the transition from observation to control. Some of these ideas could be tested using today's technology, e.g. the Advanced Photon Source or Linac Coherent Light Source, to demonstrate proof of principle and technology gaps that would need to be solved using MaRIE. Other ideas could be developed locally to demonstrate the proof-of-concept on a small scale. A series of MaRIE presentations at local seminars focused on specific topics will be scheduled in the near future, e.g. current facility definition, novel probes, needs for technology advances, etc. Attend the seminars to learn the current state of MaRIE and contact any of the leads listed above to get involved in helping define the technology needed for the MaRIE facility. In particular, we need more MST involvement in the definition of the Multi-Probe Diagnostic Hall (MPDH). If you are interested in becoming more engaged with the MPDH definition, please contact me.

MST Deputy Division Leader Dave Teter

Caro… Recruiting a senior scientist, with such a wealth of experience and proven ability, is rare for the Laboratory, according to CMIME Director Michael Nastasi.

"In my 25 years here, I have not seen it happen many times…but he was a strategic hire," said Nastasi (MST-8). Caro "is a talented guy who fills the gap needed for our research area."

CMIME is one of two Energy Frontier Research Centers at Los Alamos. These multimillion-dollar centers, funded by the Department of Energy, are enlisting the talents and skills of scientists and engineers to address the fundamental scientific roadblocks to U.S. energy security.

As a member of CMIME, Caro supports the center's mission to understand, at the atomic scale, the behavior of materials subject to extreme radiation doses and mechanical stress in order to synthesize new materials that can tolerate such conditions.

Caro said his goals as the Crystal Growth and Material Preparation team leader include using the team's intellectual resources and material capabilities to effectively coordinate the relationship between theories and experiments and to better respond as a team to funding opportunities.

"Our main purpose as scientists is to maintain the enthusiasm in doing research at the highest possible level," he said.

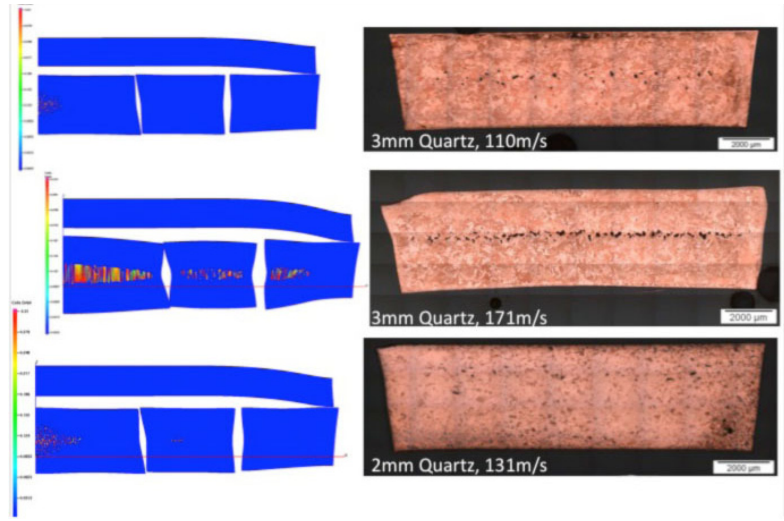
Caro's research interests include computational materials science, in particular the interface between electronic structure and the atomic scale, including the thermodynamic aspects of multicomponent systems. His models and algorithms are applied to properties of nanostructured materials and to materials under extreme conditions of irradiation and mechanical deformation.

His objective is to continue expanding the capabilities of computational materials science to predict properties of new materials, specifically for nuclear, high-temperature, and high-strength applications that would otherwise require expensive and long-term experimentation.

"The study of defects, interfaces, and phase stability under irradiation will allow us to develop materials with unprecedented performance under these extreme conditions," Caro said.

Microstructure in the extreme environment

Ellen Cerreta (Structure/Property Relations, MST-8) gave an invited talk on research into materials failure under high strain rates. The research specifically examined the connections between characteristics of loading environments and material length scales to help enhance the physics representing damage evolution within Los Alamos National Laboratory's current models. She gave her presentation at the inaugural National Security Science Seminar in Washington, D.C. The new seminar series, sponsored by the National Nuclear Security Administration's Laboratory Directed Research and Development (LDRD) program office, showcases strong connections between LDRD programs and science underpinning national security concerns.



(Left): TEPLA damage plasticity simulations of damage, and (right) dynamic experiments with post mortem characterization show the connection between small changes in loading environment and larger differences in evolved damage.

Cerreta's presentation, "Isolating the Influence of Kinetic and Spatial Effects on Dynamic Damage," elaborated on the coupled influence of dynamic loading environment and microstructure critical to accurately predicting material performance in numerous applications, including defense, aerospace, and manufacturing. Models capturing the physics of this interaction between microstructure and loading history are particularly pertinent to national security. An important first step in advancing damage models is a physical understanding of complicated dynamic deformation and failure processes.

In the research described in the talk, scientists conducted model-driven dynamic experiments using gas gun platforms to impart early stage damage to copper with varying defect distributions, in this case grain sizes. These specimens were soft recovered and examined post mortem using both two-dimensional and three-dimensional characterization techniques, including optical microscopy, scanning electron microscopy, electron back scattered

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Microstructure. . . diffraction, and x-ray tomography. The results revealed uniqueness between loading characteristics and damage evolution (see figure). For example, damage becomes more localized as peak shock pressure increases. The damage volume does not appear to depend on defect distribution, but the size distribution of voids that open within a material during a dynamic loading is highly dependent on grain size. The damage appears to have some deterministic features, and three-dimensional characterization reveals aspects of radial release and void coalescence. This type of characterization will be used to advance polycrystalline damage models to accurately capture the early stages of dynamic damage evolution.

This research is comprised of three multidisciplinary teams. The Dynamic Testing team consisted of Darcie Dennis-Koller (Shock and Detonation Physics, WX-9), and Carl Trujillo and Daniel Martinez (MST-8). The Mechanical Behavior/Microstructural Characterization Team included Cerreta, Juan Pablo Escobedo, Mike Lopez, Veronica Livescu (MST-8); Brian Patterson (Polymers and Coatings, MST-7); and TJ Ulrich (Geophysics, EES-17). The Modeling and Simulation team consisted of Curt Bronkhorst, Ben Hansen, and Hashem Mourad (Fluid Dynamics and Solid Mechanics, T-3); Ricardo Lebensohn (MST-8); and Davis Tonks and Dean Preston (Materials and Physical Data, XCP-5). The Laboratory-Directed Research and Development (LDRD) program funded the research.

Hollis assists local companies for NM Small Business Assistance program

Kendall Hollis (Materials Technology: Metallurgy, MST-6) helped two local businesses on projects as part of the New Mexico Small Business Assistance (NMSBA) program. This program enables New Mexico small businesses facing a technical challenge to access the expertise and capabilities of Los Alamos and Sandia National Laboratories. At no cost to the business, small businesses with a technical challenge can seek assistance from Laboratory scientists or engineers for projects that require testing, design consultation, and access to special equipment or facilities.

Hollis helped Doug Scott Art of Taos to investigate the production of sculpture art. Artist Doug Scott created a rubber mold in a material used traditionally for casting a wax replica of the original. Hollis sprayed metal into a mold instead of using the traditional lost wax casting method. If successful, the new process could decrease the time and cost of producing metal sculpture art while increasing the possible metals and metal combinations used to produce the art. The critical test was whether the soft molding material could withstand the heat of the sprayed molten metal and if replication of the fine details in the mold was possible in the metal deposit. Metal spraying at Los Alamos onto the artist's mold produced good replication of the mold detail without melting the mold (see photos). Hollis found that mold stiffness and curvature are important parameters to control when optimizing the process.


(Left): The artist's rubber mold (pink) with a plaster backing (white). Part of the mold was sprayed with metal to form the piece, which is shown in the photo on the right. The lines in the mold are reproduced well in the metal.

Hollis also assisted an Albuquerque-based company that needed to cure polymer coatings with portable equipment in outdoor environments. The company requested help to identify and evaluate possible commercial curing technologies that could optimize the company's specific application. Hollis investigated traditional technologies such as hot air, infrared, and ultraviolet curing. In addition, he evaluated a flame-sprayed polymer alternative and compared it with the traditional curing processes. Hollis analyzed the compiled information and made a technology recommendation to the company.

Electron backscattering diffraction enables serial number restoration

Carl Necker (MST-6) gave an invited talk on restoring serial numbers using electron backscatter diffraction (EBSD). This technique could potentially uncover forensic evidence unavailable through current techniques. The novel electron microscopy technique aids the restoration of defaced serial numbers from weapons and other items that have a key role in forensic analysis. Necker presented the research at the Microscopy and Microanalysis conference in Portland, Oregon, for the Microscopy Society of America.

The restoration process typically requires polishing and etching with a specific acid to attack the residual deformation caused by the initial impression process. Under the right conditions, the

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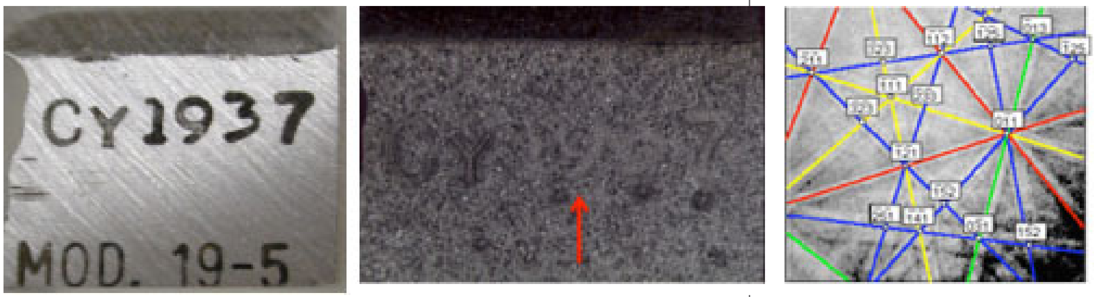

(Far left): Serial number after initial grinding step. (Center): Serial number sequence beginning with "9" has been ground away, shown in etch relief (arrow points at "9"). (Left): Typical electron backscatter diffraction pattern with calculated crystal orientation overlay. The colored bands in the overlay represent the best-fit calculated crystal orientation for that pattern.

Diffraction . . etching process provides an optical "ghost" image of the original impression.

With this new technique, Necker and Robert Forsyth (MST-6) developed the sample preparation requirements and assessed initial EBSD scan results on handgun serial numbers to determine how well the technique can recover serial numbers (see figures above, left and center). The EBSD process requires polishing and light etching or electropolishing for optimal results. The electron beam is moved through a surface array of points where the crystallographic orientation is captured at each point. The collective crystallographic information from all the patterns can be used to reconstruct the microstructure and then assess the microstructure and texture using image analysis techniques (see figure above, right). The research is in its early stages. Future studies will determine how far below the bottom of the visible impression EBSD can re-establish serial number evidence in a variety of metallic materials. Legal and forensic organizations could be interested in the EBSD technique because it may improve evidence accuracy and precision.

Celebrating service

Congratulations to the following MST Division employees celebrating service anniversaries recently:

Steven Conradson, MST-8	25 years
Anna Zurek, MST-8	25 years
James Valdez, MST-8	15 years
Beverly Basey-Jones, MST-8	5 years
Alice Smith, MST-16	5 years

HeadsUP!

Be sure to enter your T&L on time

The Associate Directorate for Experimental Physical Sciences has recently issued Oracle Time and Labor Guidance for Timekeepers that affects those who do not meet the deadline for time and labor entry. ADEPS is following CFO guidance for OTL timekeepers presented at the All Managers' Meeting September 21 by Scott Larkin, which states *"For employees who have not submitted a timecard by 9:00 a.m., instruct timekeepers to charge the employee's vacation, or leave without pay if the employee does not have sufficient accrued vacation."* For the specfic actions in this guidance, please see ADEPS 10-011 OTL Guidance for Timekeepers, at int.lanl.gov/orgs/adeps/policy.shtml.

Safe driving tips

The number one DOE activity that results in fatalities is something that everyone does each day–driving! From 1999-2009 there were 13 motor vehicle-related deaths out of 26 total DOE fatalities. More recently, from 2008-2009, there were four DOE motor vehicle-related fatalities.

DOE has many different makes and models of motor vehicles that are driven by employees in the daily performance of work. Evidence exists that drivers may not be sufficiently familiar with the operating controls and other features of a vehicle before they adjust them while driving. Being distracted (searching for unfamiliar vehicle controls) while operating a motor vehicle is the surest way to have an accident. Many long-term university research projects have consistently demonstrated that distracted driving affects reaction times in a manner that is similar to driving under the influence of drugs or alcohol. In the October 2010 Office of Health, Safety and Security Just-in-Time Report on this topic, several cases, one a fatality, are described that involved drivers trying to find the parking brake release lever on government vehicles they were operating. The simpliest task can turn deadly in unfamiliar settings.

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